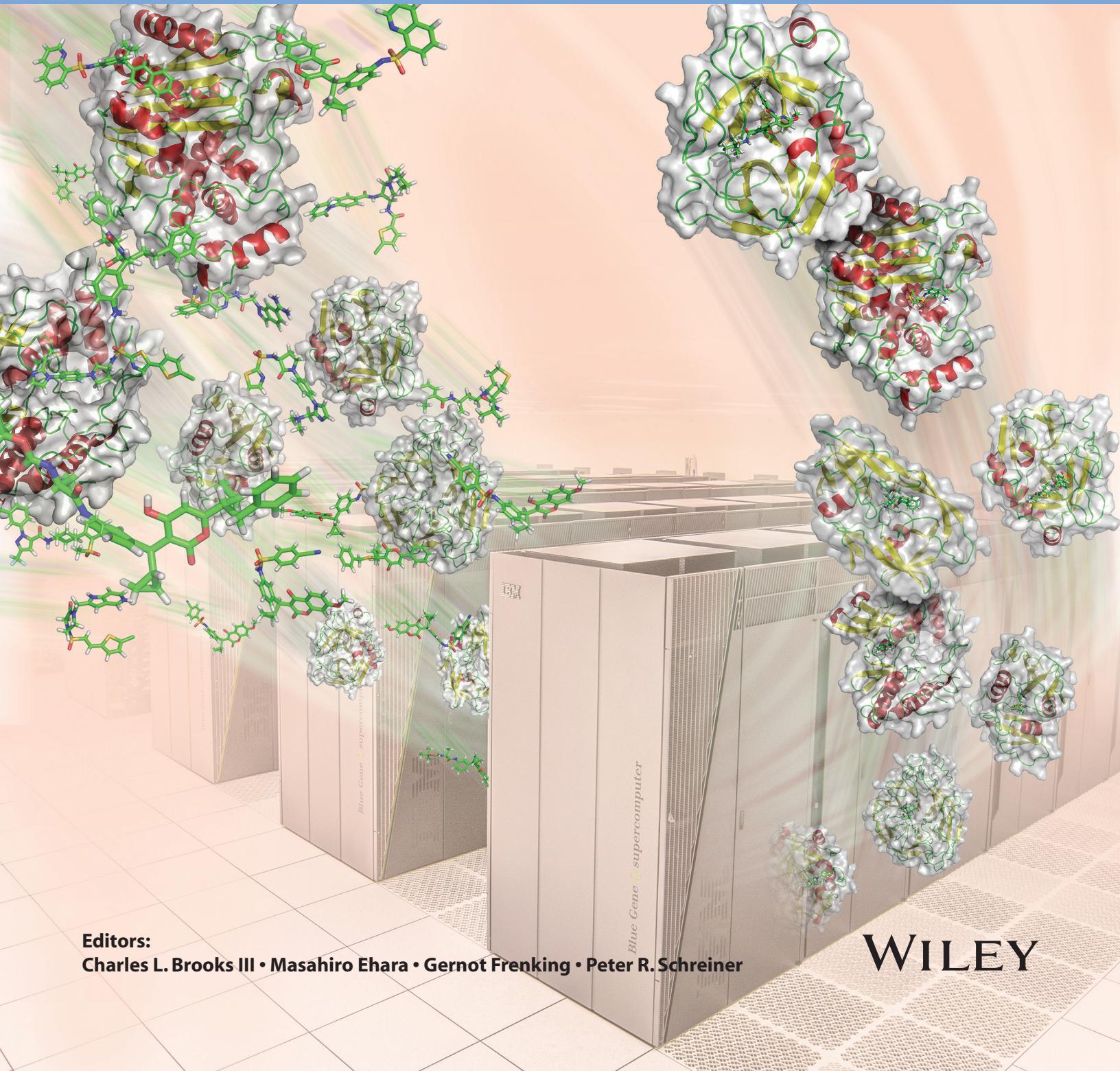


Volume 34 | Issues 11–12 | 2013  
Included in this print edition:  
Issue 11 (April 30, 2013)  
Issue 12 (May 5, 2013)

# Journal of COMPUTATIONAL CHEMISTRY

Organic • Inorganic • Physical  
Biological • Materials

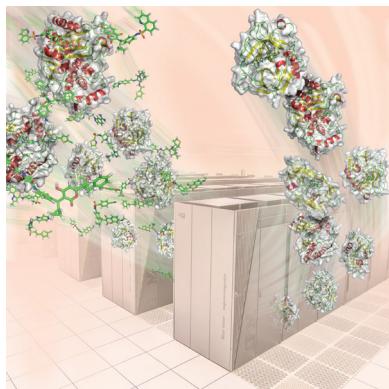
[www.c-chem.org](http://www.c-chem.org)



Editors:

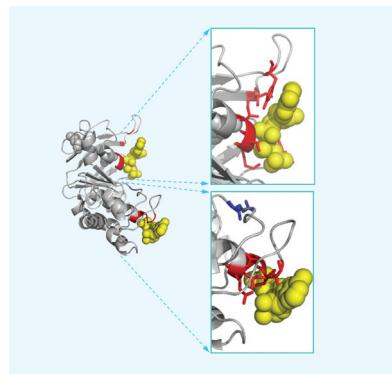
Charles L. Brooks III • Masahiro Ehara • Gernot Frenking • Peter R. Schreiner

WILEY



## Parallel Molecular Docking

The front cover illustrates the parallel molecular docking of large databases on the Sequoia, a petascale IBM Blue Gene/Q supercomputer at Lawrence Livermore National Laboratory. A mixed parallel scheme that combines MPI and multithreading is implemented by Xiaohua Zhang, Sergio E. Wong, and Felice C. Lightstone on page 915 in the Vina molecular docking program named VinaLC, where LC stands for Livermore Computing. Parallel performance analysis shows the code scales up to more than 15K CPUs with a very low overhead cost of 3.94%. One million flexible compound docking calculations take only 1.4 hours on about 15K CPUs. The picture shows ligands that have been docked into various receptors to form ligand–receptor complexes via calculations on the Sequoia.



## ATP Binding Site Prediction

TargetATPsite, a new method based on residue evolution image sparse representation and classifier ensemble, is developed for predicting ATP-binding sites from primary sequences, as presented by Dong-Jun Yu, Jun Hu, Yan Huang, Hong-Bin Shen, Yong Qi, Zhen-Min Tang, and Jing-Yu Yang on page 974. The high performance of TargetATPsite originates from the good discriminative capability of the new image sparse representation feature and the power of the modified AdaBoost classifier ensemble. TargetATPsite also features the capability of further identifying the binding pockets from the predicted binding residues through a spatial clustering algorithm.

## Coming Soon

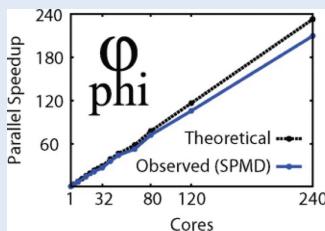
Look for these important papers  
in upcoming issues

**PHI:** A powerful new program for the analysis of anisotropic monomeric and exchange-coupled polynuclear *d*- and *f*-block complexes

Keith S. Murray et al.

A new and extensively parallelized code for the calculation of the magnetic properties of large spin systems or complex orbitally degenerate compounds is presented. The program can simulate theoretical systems or fit experimental data with a specific Hamiltonian.

DOI: 10.1002/jcc.23234



Parameterization of a reactive force field using a Monte Carlo algorithm

C. C. M. Rindt et al.

Parameterization of a reactive force field (ReaxFF) is performed using a robust Metropolis Monte Carlo algorithm for a system of magnesium sulfate hydrates. This new method for optimizing the force field is efficient especially without good initial conditions. The stochastic nature enables one to arrive at the global minimum in the parameter space and thereby the best obtainable force field.

DOI: 10.1002/jcc.23246

